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# Commuting self-adjoint extensions of symmetric operators defined from the partial derivatives

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We consider the problem of finding commuting self-adjoint extensions of the partial derivatives  $\{(1/i)(\partial/\partial x_j): j=1,\dots,d\}$  with domain  $C_c^\infty(\Omega)$  where the self-adjointness is defined relative to  $L^2(\Omega)$ , and  $\Omega$  is a given open subset of  $\mathbb{R}^d$ . The measure on  $\Omega$  is Lebesgue measure on  $\mathbb{R}^d$  restricted to  $\Omega$ . The problem originates with Segal and Fuglede, and is difficult in general. In this paper, we provide a representation-theoretic answer in the special case when  $\Omega = I \times \Omega_2$  and  $I$  is an open interval. We then apply the results to the case when  $\Omega$  is a  $d$  cube,  $I^d$ , and we describe possible subsets  $\Lambda \subset \mathbb{R}^d$  such that  $\{e_\lambda|_{I^d}: \lambda \in \Lambda\}$  is an orthonormal basis in  $L^2(I^d)$ . © 2000 American Institute of Physics. [S0022-2488(00)02712-2]

## I. INTRODUCTION

Recently several papers have appeared on commuting non-self-adjoint operators and their spectral theory; see, e.g., Ref. 1. The present paper concerns the case when the given commuting operators are unbounded and symmetric, but non-self-adjoint. A concrete class of operators is studied, and we address the questions of when commuting extension operators exist and, when they do exist, what their structural properties are.

The problem of understanding commuting symmetric, but non-self-adjoint, unbounded operators also has an origin in mathematical physics.<sup>2-5</sup> The terminology from physics is “Hermitian,” or “*formally* self-adjoint,” for symmetry, i.e., for the identity  $\langle Sf|h \rangle = \langle f|Sh \rangle$  for all vectors  $f, h$  in the domain of the operator  $S$ . The simplest case of this is the problem of assigning quantum mechanical boundary conditions for free particles confined in a box. More specifically, the problem here corresponds to the quantum-mechanical trajectories of a particle confined to a region of tube type, e.g., a unit cube. It is “free” except for the boundary conditions, and variations of the boundary conditions (as considered here) correspond to different physics. For single operators, von Neumann solved (or made precise) the problem by use of the Cayley transform, and considering instead the extension problem for partial isometries. But this approach does not work well in the case of several operators. Powers (in Refs. 6 and 7) introduced an algebraic approach for understanding several operators, but the present problem is very concrete and does not lend itself easily to the algebraic techniques introduced by Powers.

Closely connected to the problem of finding commuting self-adjoint extensions of  $(1/i)(\partial/\partial x_j)$ ,  $j=1,\dots,d$ , on  $C_c^\infty(\Omega)$  is the corresponding spectral question: If commuting self-adjoint extensions do exist, then it is known that the common eigenfunctions of the extension operators must be of the form  $e_\lambda := e^{i\lambda \cdot x}$  for special values of  $\lambda \in \mathbb{R}^d$ . Hence the spectral problem is that of finding when a given pair  $(\Omega, \Lambda)$  satisfies the condition that  $\{e_\lambda|_\Omega: \lambda \in \Lambda\}$  is an orthogonal basis in the Hilbert space  $L^2(\Omega)$ . We note that this so-called *spectral pair* condition is very restrictive, and so it explains the rigid geometric configurations  $(\Omega, \Lambda)$  which admit solutions. But

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it also serves to motivate recent very interesting developments on overcomplete systems; see, e.g., Refs. 8 and 9.

The setting of *spectral pairs* in  $d$  real dimensions involves two subsets  $\Omega$  and  $\Lambda$  in  $\mathbb{R}^d$  such that  $\Omega$  has finite and positive  $d$ -dimensional Lebesgue measure, and  $\Lambda$  is an index set for an orthogonal  $\mathcal{L}^2(\Omega)$ -basis  $e_\lambda$  of exponentials, i.e.,

$$e_\lambda(x) = e^{i2\pi\lambda \cdot x}, \quad x \in \Omega, \quad \lambda \in \Lambda, \quad (1.1)$$

where  $\lambda \cdot x = \sum_{j=1}^d \lambda_j x_j$ . We use vector notation  $x = (x_1, \dots, x_d)$ ,  $\lambda = (\lambda_1, \dots, \lambda_d)$ ,  $x_j, \lambda_j \in \mathbb{R}$ ,  $j = 1, \dots, d$ . The basis property refers to the Hilbert space  $\mathcal{L}^2(\Omega)$  with inner product

$$\langle f | g \rangle_\Omega := \int_\Omega \overline{f(x)} g(x) dx, \quad (1.2)$$

where  $dx = dx_1 \cdots dx_d$ , and  $f, g \in \mathcal{L}^2(\Omega)$ . The corresponding norm is

$$\|f\|_\Omega^2 := \langle f | f \rangle_\Omega = \int_\Omega |f(x)|^2 dx, \quad (1.3)$$

as usual. It follows that the spectral pair property for a pair  $(\Omega, \Lambda)$  is equivalent to

$$\Lambda - \Lambda = \{\lambda - \lambda' : \lambda, \lambda' \in \Lambda\}$$

being contained in the *zero-set* of the complex function

$$z \mapsto \int_\Omega e^{i2\pi z \cdot x} dx =: F_\Omega(z), \quad (1.4)$$

where  $z = (z_1, \dots, z_d) \in \mathbb{C}^d$ , and  $z \cdot x := \sum_{j=1}^d z_j x_j$ , and the corresponding  $e_\lambda$ -set  $\{e_\lambda : \lambda \in \Lambda\}$  being *total* in  $\mathcal{L}^2(\Omega)$ . Recall, totality means that the span of the  $e_\lambda$ 's is dense in  $\mathcal{L}^2(\Omega)$  relative to the  $\|\cdot\|_\Omega$ -norm, or, equivalently, that  $f=0$  is the only  $\mathcal{L}^2(\Omega)$ -solution to

$$\langle f | e_\lambda \rangle_\Omega = 0, \quad \text{for all } \lambda \in \Lambda.$$

## II. SPECTRAL PAIRS

The theory of *spectral pairs* was developed in previous joint papers by the coauthors.<sup>10–12</sup> A set  $\Omega$  with finite nonzero Lebesgue measure is called a *spectral set* if  $(\Omega, \Lambda)$  is a spectral pair for some set  $\Lambda$ . We recall that Fuglede showed<sup>13</sup> that the disk and the triangle in two dimensions are *not spectral sets*. By the disk and the triangle we mean the usual versions, respectively,  $\{(x_1, x_2) \in \mathbb{R}^2 : x_1^2 + x_2^2 < 1\}$  and  $\{(x_1, x_2) \in \mathbb{R}^2 : 0 < x_1, 0 < x_2, x_1 + x_2 < 1\}$ . Note that, for the present discussion, it is inessential whether or not the sets  $\Omega$  are taken to be open, but it is essential for the following theorem which we will need. It is due to Fuglede and the coauthors; see Refs. 10, 13–15.

If  $\Omega \subset \mathbb{R}^d$  is open, then we consider the partial derivatives  $\partial/\partial x_j$ ,  $j = 1, \dots, d$ , defined on  $C_c^\infty(\Omega)$  as unbounded skew-symmetric operators in  $\mathcal{L}^2(\Omega)$ . The corresponding versions  $(1/2\pi\sqrt{-1})(\partial/\partial x_j)$  are symmetric of course. We say that  $\Omega$  has the *extension property* if there are commuting self-adjoint extension operators  $H_j$ , i.e.,

$$\frac{1}{2\pi i} \frac{\partial}{\partial x_j} \subset H_j, \quad j = 1, \dots, d. \quad (2.1)$$

We say that the containment  $A \subset B$  holds for two operators  $A$  and  $B$  if the graph of  $A$  is contained in that of  $B$ . (For details, see Refs. 16 and 17.) *Commutativity* for the extension operators  $H_j$  is in

the strong sense of spectral resolutions. Since the  $H_j$ 's are assumed self-adjoint, each one has a projection-valued *spectral resolution*  $E_j$ , i.e., an  $\mathcal{L}^2(\Omega)$ -projection-valued Borel measure on  $\mathbb{R}$ , such that  $E_j(\mathbb{R}) = I_{\mathcal{L}^2(\Omega)}$ , and

$$H_j = \int_{-\infty}^{\infty} \lambda E_j(d\lambda) \quad (2.2)$$

for  $j = 1, \dots, d$ . The strong commutativity is taken to mean

$$E_j(\Delta)E_{j'}(\Delta') = E_{j'}(\Delta')E_j(\Delta) \quad (2.3)$$

for all  $j, j' = 1, \dots, d$ , and all Borel subsets  $\Delta, \Delta' \subset \mathbb{R}$ . Extensions commuting in a weaker sense were considered in Ref. 18.

Our analysis is based on von Neumann's deficiency-space characterization of the self-adjoint extensions of a given symmetric operator.<sup>19</sup> Let  $\Omega$  be an open set with finite Lebesgue measure. For each  $j$ , the deficiency spaces corresponding to  $(1/i)(\partial/\partial x_j)$  are infinite dimensional. It follows that each  $(1/i)(\partial/\partial x_j)$  has "many" self-adjoint extensions. The main problem (not addressed by von Neumann's theory) is the selection of a commuting set  $H_1, H_2, \dots, H_d$  of extensions. In fact, for some  $\Omega$  (e.g., when  $d=2$ , the disk and the triangle) it is impossible to select a commuting set  $H_1, H_2, \dots, H_d$  of extensions.

We have (see Refs. 10, 13–15)

**Theorem II.1 (Fuglede, Jorgensen, Pedersen):** *Let  $\Omega \subset \mathbb{R}^d$  be open and connected with finite and positive Lebesgue measure. Then  $\Omega$  has the extension property if and only if it is a spectral set. Moreover, with  $\Omega$  given, there is a one-to-one correspondence between the two sets of subsets:*

$$\{\Lambda \subset \mathbb{R}^d: (\Omega, \Lambda) \text{ is a spectral pair}\} \quad (2.4)$$

and

$$\{\Lambda \subset \mathbb{R}^d: \Lambda \text{ is the joint spectrum of some}$$

$$\text{commutative family } (H_1, \dots, H_d) \text{ of self-adjoint extensions}\}. \quad (2.5)$$

This correspondence is determined as follows:

(a) If the extensions  $(H_1, \dots, H_d)$  are given, then  $\lambda \in \Lambda$  if and only if

$$e_\lambda \in \bigcap_j \text{domain } (H_j). \quad (2.6)$$

(b) If, conversely,  $(\Omega, \Lambda)$  is a spectral pair at the outset, then the ansatz (2.6) and

$$H_j e_\lambda = \lambda_j e_\lambda, \quad \lambda \in \Lambda \quad (2.7)$$

determine uniquely a set of commuting extensions.

If  $\Omega$  is only assumed open, then the spectral-set property implies the extension property, but not conversely.

**Corollary II.2:** *Suppose  $\Omega$  is open and connected. It follows then that a discrete set  $\Lambda$  is the joint spectrum of some commuting self-adjoint extension operators  $H_j, j=1, \dots, d$ , if and only if  $(\Omega, \Lambda)$  is a spectral pair.*

**Remark II.3:** The simplest case of a disconnected  $\Omega$  which has the extension property, but which is not a spectral set, is in  $d=1$ , and we may take  $\Omega = \langle 0, 1 \rangle \cup \langle 2, 4 \rangle$ , i.e., the union of two intervals with a doubling and separation. The example was noted first in Ref. 13 and is based on the simple observation that the polynomial  $1 + z^2 + z^3$  has no roots  $z$  on the circle  $|z|=1$ .

Some of the interest in spectral pairs derives from their connection to *tilings*. A subset  $\Omega \subset \mathbb{R}^d$  with nonzero measure is said to *tile*  $\mathbb{R}^d$  if there is a set  $L \subset \mathbb{R}^d$  such that the translates  $\{\Omega + l : l \in L\}$  cover  $\mathbb{R}^d$  up to measure zero, and if the intersections

$$(\Omega + l) \cap (\Omega + l') \quad \text{for } l \neq l' \text{ in } L \quad (2.8)$$

have measure zero. We will call  $(\Omega, L)$  a *tiling pair* and we will say that  $L$  is a *set of translations*. The *spectral-set conjecture* (see Refs. 13–15, 20, 21) states:

**Conjecture II.4:** Let  $\Omega \subset \mathbb{R}^d$  have positive and finite Lebesgue measure. Then  $\Omega$  is a spectral set if and only if there is a set  $L$  of translations which make  $\Omega$  tile  $\mathbb{R}^d$ .

**Lemma II.5:** If  $\Omega = I^d$ , then the zero set for the function  $F_\Omega$  in (1.4) is

$$\mathbf{Z}_{I^d} = \{z \in \mathbb{C}^d \setminus \{0\} : \exists j \in \{1, \dots, d\} \text{ s.t. } z_j \in \mathbb{Z} \setminus \{0\}\}. \quad (2.9)$$

*Proof:* The function  $F_{I^d}(\cdot)$  factors as follows:

$$F_{I^d}(z) = \prod_{j=1}^d e^{i\pi z_j} \frac{\sin \pi z_j}{\pi z_j} \quad (2.10)$$

for  $z = (z_1, \dots, z_d) \in \mathbb{C}^d$ , with the interpretation that the function  $z \mapsto (\sin \pi z)/\pi z$  is 1 when  $z = 0$  in  $\mathbb{C}$ .  $\square$

**Remark II.6:** What is special about  $\mathbf{Z}_\Omega$  for  $\Omega = I^d$ , as opposed to the general form of  $\Omega$ , is that  $\mathbf{Z}_{I^d} \cup \{0\}$  is the Cayley graph of the group  $\Gamma = \mathbb{Z}^d$  with generators

$$S = \{(\pm 1, 0, \dots, 0), \dots, (0, \dots, \pm 1, 0, \dots, 0), \dots, (0, \dots, 0, \pm 1)\}.$$

We recall from Ref. 22, Chapter 10, the definition of the Cayley graph  $G(\Gamma, S)$  of a discrete group  $\Gamma$  with generators  $S$ ,  $e \notin S$ . When  $\Gamma, S$  are given,  $G(\Gamma, S)$  is the graph with vertex set  $\Gamma$  in which two vertices  $\gamma_1, \gamma_2$  are the two ends of an edge iff  $\gamma_1^{-1} \gamma_2 \in S$ . This gives a nonoriented graph, without any loop or multiple edge.

### III. TWO DIMENSIONS

We begin with the following simple observation in one dimension for  $\Omega = I = [0, 1)$ . (For details, see Refs. 10 and 16.)

**Proposition III.1:** The only subsets  $\Lambda \subset \mathbb{R}$  such that  $(I, \Lambda)$  is a spectral pair are the translates

$$\Lambda_\alpha := \alpha + \mathbb{Z} = \{\alpha + n : n \in \mathbb{Z}\}, \quad (3.1)$$

where  $\alpha$  is some fixed real number.

In two dimensions, the corresponding result is more subtle, but the possibilities may still be enumerated as follows:

**Theorem III.2 (Ref. 23):** The only subsets  $\Lambda \subset \mathbb{R}^2$  such that  $(I^2, \Lambda)$  is a spectral pair must belong to either one or the other of the two classes, indexed by a number  $\alpha$ , and a sequence  $\{\beta_m \in [0, 1) : m \in \mathbb{Z}\}$ , where

$$\Lambda = \left\{ \begin{pmatrix} \alpha + m \\ \beta_m + n \end{pmatrix} : m, n \in \mathbb{Z} \right\} \quad (3.2)$$

or

$$\Lambda = \left\{ \begin{pmatrix} \beta_n + m \\ \alpha + n \end{pmatrix} : m, n \in \mathbb{Z} \right\}. \quad (3.3)$$

Each of the two types occurs as the spectrum of a pair for the cube  $I^2$ , and each of the sets  $\Lambda$  as specified is a set of translation vectors which produces a tiling of  $\mathbb{R}^2$  by the cube  $I^2$ .

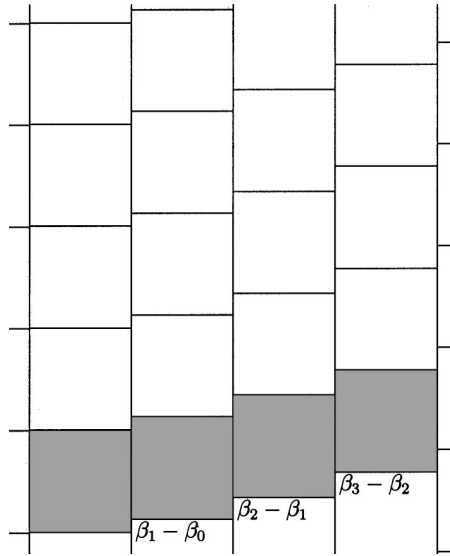


FIG. 1. Illustrating tiling with (3.2).

*Proof:* See Ref. 23 for details. The following are some remarks of relevance to the general extension problem for operators.

The assertion in the theorem about  $\Lambda$  translations tiling the plane with  $I^2$  is also clear from (3.2) and (3.3), and is illustrated graphically in Figs. 1 and 2.

It is clear that the pattern (3.2) for  $d=2$  continues to higher dimensions as follows:

$$\begin{pmatrix} \alpha + k_1 \\ \beta(k_1) + k_2 \\ \gamma(k_1, k_2) + k_3 \\ \vdots \\ \zeta(k_1, k_2, \dots, k_{d-1}) + k_d \end{pmatrix} \quad (3.4)$$

with  $k_1, k_2, \dots, k_d \in \mathbb{Z}$ , and

$$\begin{aligned} \beta: \mathbb{Z} &\rightarrow [0, 1), \\ \gamma: \mathbb{Z} \times \mathbb{Z} &\rightarrow [0, 1), \\ &\vdots \\ \zeta: \mathbb{Z}^{d-1} &\rightarrow [0, 1). \end{aligned}$$

Of course, then there are the obvious modifications of those cases resulting from permutation of the  $d$  coordinates; but the assertion is that, when  $d \geq 10$ , these configurations do not suffice for cataloguing all the possible spectra  $\Lambda$  which turn  $(I^d, \Lambda)$  into an  $\mathbb{R}^d$ -spectral pair.

We now turn to the nontrivial spectral-theoretic content of the conclusion of the theorem. We claim that the two cases (3.2) and (3.3) suffice when  $d=2$ . Note that the sequence  $\beta: \mathbb{Z} \rightarrow [0, 1)$  is completely arbitrary.

We will show in Theorem V.1 that, up to a single translation in the plane, the possibilities for the coordinates of points in a spectrum  $\Lambda$  for  $I^2$  are given by two sequences  $\xi_m, \eta_n$  satisfying the following two cocycle relations:

$$(e^{i\xi_{m+k}} - e^{i\xi_m})(1 - e^{i\eta_n}) = 0 \quad (3.5)$$

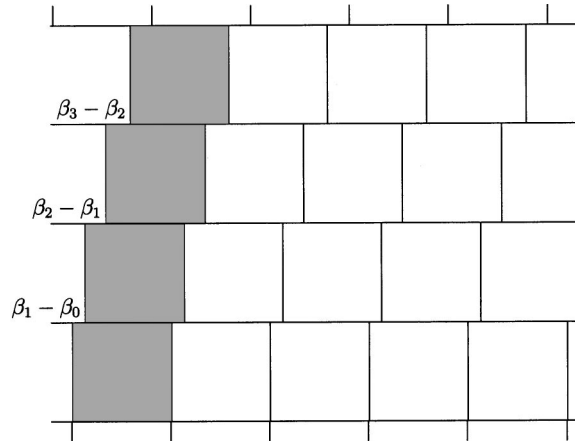


FIG. 2. Illustrating tiling with (3.3).

and

$$(e^{i\eta_{n+l}} - e^{i\eta_n})(1 - e^{i\xi_m}) = 0 \quad (3.6)$$

as identities in  $m, n \in \mathbb{Z}$ , and  $k, l \in \mathbb{Z} \setminus \{0\}$ . Note that the respective sequences are determined from this only up to  $2\pi\mathbb{Z}$  at each coordinate place.

Simple algebra shows that the two identities (3.5) and (3.6) imply the following single identity:

$$(1 - e^{i\xi_{m+k}})(1 - e^{i\eta_n}) = (1 - e^{i\xi_m})(1 - e^{i\eta_{n+l}}) \quad (3.7)$$

again for all  $m, n \in \mathbb{Z}$  and  $k, l \in \mathbb{Z} \setminus \{0\}$ . But it follows from (3.7) that at least one of the two sequences,  $1 - e^{i\xi_m}$  or  $1 - e^{i\eta_n}$ , must then vanish identically. This yields the connection to the two cases for  $\Lambda$  stated in (3.2) and (3.3) of the theorem.

Hence the result giving two classes for  $\Lambda$  in Theorem III.2 may be derived from our more general result in Sec. V.

The proof sketch of Theorem III.2 is completed for now, but details will be resumed in Sec. V.  $\square$

#### IV. OPERATOR EXTENSIONS

We saw in Theorem II.1 that in some cases the existence problem for spectral pairs, i.e., the question of when some given open subset  $\Omega$  in  $\mathbb{R}^d$  has an orthogonal basis  $\{e_\lambda : \lambda \in \Lambda\}$  in  $\mathcal{L}^2(\Omega)$  for some set  $\Lambda$  in  $\mathbb{R}^d$ , may be reformulated as a problem about existence of commuting self-adjoint extensions of the operators  $\{(1/i)(\partial/\partial x_j) : j=1, \dots, d\}$  with common (dense) domain  $C_c^\infty(\Omega)$  in  $\mathcal{L}^2(\Omega)$ . Suppose for the moment that  $\Omega = \langle 0, 1 \rangle \times \Omega_2$  where  $\Omega_2$  is some subset in  $\mathbb{R}^{d-1}$  of finite positive  $(d-1)$ -dimensional Lebesgue measure. We then have the following classification of the self-adjoint extensions  $H$  of  $(1/i)(\partial/\partial x_1)$ .

**Theorem IV.1:** *The symmetric operator  $(1/i)(\partial/\partial x_1)$  in  $\mathcal{L}^2(\langle 0, 1 \rangle \times \Omega_2)$  with dense domain  $\mathcal{D}$  consisting of  $\varphi \in \mathcal{L}^2(\langle 0, 1 \rangle \times \Omega_2)$  such that  $\varphi(\cdot, y) \in C_c^\infty(\langle 0, 1 \rangle)$  for all  $y \in \Omega_2$ , has self-adjoint extensions indexed by unitary operators  $V$  in  $\mathcal{L}^2(\Omega_2)$  in such a way that the (unique) extension  $H_V$  is determined by its core domain being of the form*

$$\mathcal{D}_V = \{\varphi(x_1, y) + e^{x_1}h(y) + e^{1-x_1}(Vh)(y) : \varphi \in \mathcal{D}, h \in \mathcal{L}^2(\Omega_2)\} \quad (4.1)$$

and

$$iH_V(\varphi + e^{x_1}h + e^{1-x_1}Vh) = \frac{\partial \varphi}{\partial x_1} + e^{x_1}h - e^{1-x_1}Vh, \quad (4.2)$$

for  $\varphi \in \mathcal{D}$  and  $h \in \mathcal{L}^2(\Omega_2)$ . We shall interpret the implicit boundary condition dictating some extension  $H_V$  as

$$f(1, \cdot) = U_V(f(0, \cdot)), \quad (4.3)$$

$f \in \mathcal{D}_V$  where the partial isometry  $U_V$  is given by

$$W_V = (eI + V)(I + eV)^{-1}, \quad U_V = \exp W_V. \quad (4.4)$$

Conversely,  $V$  may be calculated from  $U_V$  by

$$V = (I - eW_V)^{-1}(W_V - eI), \quad (4.5)$$

and in each case, the fractional linear transform, and its inverse, are well defined.

*Proof:* The proof is based on von Neumann's deficiency-space analysis of self-adjoint extensions, and we refer to Refs. 16, 19, and 24 for background material on the theory of operator extensions. If  $S$  is a symmetric operator with dense domain  $\mathcal{D}$  in a Hilbert space  $\mathcal{H}$ , then it has self-adjoint extension if and only if the two spaces

$$((iI \pm S)\mathcal{D})^\perp =: \mathcal{D}_\pm \quad (4.6)$$

have the same dimensions. In that case, the corresponding extensions are given by *partial isometries* between the respective defect spaces  $\mathcal{D}_+$  and  $\mathcal{D}_-$  (see Ref. 16, 17, or 19). For convenience, we have chosen a slightly different “normalization” in our treatment of the Cayley transform (4.4) and its inverse (4.5). We did not normalize the functions  $e^{x_1}$  and  $e^{1-x_1}$  in the defect spaces. They have  $\mathcal{L}^2(I)$ -norm equal to

$$\left( \frac{e^2 - 1}{2} \right)^{1/2}.$$

The fact that  $U_V$  in (4.4) then defines a partial isometry as claimed amounts to the identities:

If  $\psi(x_1, y) = e^{x_1}h(y) + e^{1-x_1}(Vh)(y)$  as in (4.1), then

$$\psi(1, y) = eh(y) + (Vh)(y) = (eI + V)h,$$

and

$$\psi(0, y) = h(y) + eVh(y) = (I + eV)h.$$

This means that the vectors in the domain (4.1) are given by the boundary conditions (4.3) which in turn determine the unitary one-parameter group

$$\mathcal{U}_V(t) := \exp(itH_V), \quad t \in \mathbb{R}.$$

This group is defined from (4.3) by using translation modulo  $\mathbb{Z}$  in the  $x_1$  variable. Then the operator  $U_V$  in (4.4) is used in defining the representation  $\mathbb{R} \ni t \mapsto \mathcal{U}_V(t)$  via induction from  $\mathbb{Z}$ .

If  $V: \mathcal{D}_+ \rightarrow \mathcal{D}_-$  is a partial isometry, then the domain of the corresponding extension  $H(H = H_V)$  is

$$\{\varphi + h_+ + Vh_+ : \varphi \in \mathcal{D}, h_+ \in \mathcal{D}_+\}$$

and



$$iH_V(\varphi + h_+ + Vh_+) = iS\varphi + h_+ - Vh_+. \quad (4.7)$$

It follows that the lemma amounts to an identification of the *defect spaces*  $\mathcal{D}_\pm$  when the symmetric operator is as specified. When the variables in  $\Omega = \langle 0, 1 \rangle \times \Omega_2$  are separated as  $(x_1, y)$ ,  $0 < x_1 < 1$ ,  $y = (x_2, \dots, x_d) \in \Omega_2$ , then vectors  $h_\pm \in \mathcal{D}_\pm$  are precisely the solutions to

$$S^*h_\pm = \pm ih_\pm. \quad (4.8)$$

This amounts to solving

$$\frac{\partial}{\partial x_1} h_\pm(x_1, y) = \pm h_\pm(x_1, y)$$

in the sense of distributions, but with the restrictions  $h_\pm \in \mathcal{L}^2(\langle 0, 1 \rangle \times \Omega_2)$ . The result of the lemma then follows from von Neumann's characterization. If the minimal operator is not closed at the outset, then the resulting self-adjoint extension comes from passing to the operator closure in the formulas (4.2) and (4.7).  $\square$

*Corollary IV.2:* Let  $V$  be a unitary operator in  $\mathcal{L}^2(\Omega_2)$  and let  $H_V$  be the self-adjoint extension operator described in Theorem IV.1 in (4.2) and (4.3). Then  $H_V$  generates a unitary one-parameter group  $\{U_V(t) : t \in \mathbb{R}\}$  in  $\mathcal{L}^2(\langle 0, 1 \rangle \times \Omega_2)$  which may be realized (up to unitary equivalence) in the Hilbert space  $\mathcal{H}_V$  of measurable functions  $f : \mathbb{R} \rightarrow \mathcal{L}^2(\Omega_2)$ , satisfying

$$f(x_1 + 1) = U_V(f(x_1)), \quad (4.9)$$

for all  $x_1 \in \mathbb{R}$ , where  $U_V$  is the operator from (4.4) in Theorem IV.1, and the norm on  $\mathcal{H}_V$  is defined by

$$\|f\|_{\mathcal{H}_V}^2 = \int_0^1 \|f(x_1)\|_{\mathcal{L}^2(\Omega_2)}^2 dx_1.$$

In this space the group  $U_V(t) : \mathcal{H}_V \rightarrow \mathcal{H}_V$  is given by

$$(U_V(t)f)(x_1) = f(x_1 - t) \quad \text{for } x_1, t \in \mathbb{R}. \quad (4.10)$$

The unitary isomorphism of  $\mathcal{H}_V$  onto  $\mathcal{L}^2(\langle 0, 1 \rangle \times \Omega_2) = \mathcal{L}^2(\langle 0, 1 \rangle, \mathcal{L}^2(\Omega_2))$  is simply the restriction to  $\langle 0, 1 \rangle$  in the  $x_1$ -variable. Finally, if  $U_V(t)$  is computed in  $\mathcal{L}^2(\langle 0, 1 \rangle \times \Omega_2)$ , the formula is

$$(U_V(t)f)f(x_1, \cdot) = \begin{cases} f(x_1 - t, \cdot) & \text{if } 0 \leq t < x_1 < 1 \\ U_V(f(x_1 - t, \cdot)) & \text{if } 0 < x_1 \leq t \leq 1 \end{cases} \quad (4.11)$$

*Proof:* The realization on the space  $\mathcal{H}_V$  is the interpretation of  $U_V$  as a unitary representation of the group  $\mathbb{R}$  which is induced from the subgroup  $\mathbb{Z}$  via formula (4.10). The advantage of this viewpoint is that the spectral resolution of the unitary operator  $U_V$  leads directly to an associated direct integral decomposition for the unitary one-parameter group  $\{U_V(t) : t \in \mathbb{R}\}$  which is generated by the extension operator  $H_V$ .  $\square$

When the corollary is applied to  $\mathcal{L}^2(I \times I)$  from Sec. III we note that the respective unitary one-parameter groups,  $U_x(s)$  and  $U_y(t)$ , on  $\mathcal{L}^2(I^2)$  which are generated by self-adjoint extension operators of  $(1/i)(\partial/\partial x)$  and  $(1/i)(\partial/\partial y)$  with domain  $C_c^\infty(I^2)$ , are induced representations in the sense of (4.9) and (4.10). For the extensions of  $(1/i)(\partial/\partial x)$ , the boundary-unitary from (4.9) is acting on  $\mathcal{L}^2(\{0 < y < 1\})$ . But we shall view it as a unitary operator in  $\mathcal{L}^2(I \times I) = \mathcal{L}^2(I_x) \otimes \mathcal{L}^2(I_y)$  via  $U \leftrightarrow I \otimes U_2$  with  $U_2$  acting in the  $y$  variable. A similar observation applies to the unitary one-parameter group  $\{U_y(t) : t \in \mathbb{R}\}$  acting on  $\mathcal{L}^2(I^2)$  and generated by one of the self-adjoint extensions of  $(1/i)(\partial/\partial y)$ . Hence the boundary conditions for  $\{U_x(s) : s \in \mathbb{R}\}$  are given

by a unitary  $U \simeq I \otimes U_2$  with  $U_2$  acting in the second variable, while those of  $\{U_y(t) : t \in \mathbb{R}\}$  are determined by a second unitary operator  $V$  in  $\mathcal{L}^2(I^2)$ , now of the form  $V \leftrightarrow V_1 \otimes I$  with  $V_1$  acting in the first variable of  $\mathcal{L}^2(I \times I)$ .

With this terminology we have the following preliminary result for the square  $I^2$  in the plane.

**Theorem IV.3:** *Let  $U_x(s)$  be the unitary one-parameter group on  $\mathcal{L}^2(I \times I)$ , and let  $U_2$  be the corresponding unitary boundary operator acting in the second variable  $y$ . Then  $U_2$  commutes with the phase-periodic translation in the  $y$  variable for a phase angle  $\beta$  if and only if there is a real-valued sequence  $\{\varphi_n : n \in \mathbb{Z}\}$  such that*

$$U_x(s)e_{m+\varphi_n} \otimes e_{n+\beta} = e^{i2\pi(m+\varphi_n)s} e_{m+\varphi_n} \otimes e_{n+\beta} \quad (4.12)$$

for all  $s \in \mathbb{R}$  and  $m, n \in \mathbb{Z}$ , where for  $(\xi, \eta) \in \mathbb{R}^2$ ,  $e_\xi \otimes e_\eta(x, y) = e_\xi(x)e_\eta(y) = e^{i2\pi(\xi x + \eta y)}$ , restricted to  $(x, y) \in I^2$ .

*Proof:* Recall that some fixed unitary one-parameter group  $\{U_x(s) : s \in \mathbb{R}\}$  on  $\mathcal{L}^2(I \times I)$  is determined uniquely by the corresponding boundary operator  $I \otimes U_2$ . But it follows from Proposition III.1 that  $U_2$  satisfies the commutativity property of the theorem if and only if it is diagonalized by the basis functions  $\{e_{n+\beta} : n \in \mathbb{Z}\}$  in  $\mathcal{L}^2(I_y)$  for some  $\beta \in [0, 1)$ , i.e., if, for some sequence  $\varphi_n$ ,

$$(U_2 e_{n+\beta})(y) = e^{i2\pi\varphi_n} e_{n+\beta}(y). \quad (4.13)$$

But, according to Corollary IV.2, this means that  $U_x(s)$  as an induced representation decomposes accordingly, which is to say that the basis vectors  $e_{m+\varphi_n} \otimes e_{n+\beta}$  simultaneously diagonalize each operator  $U_x(s)$  as stated in formula (4.12).  $\square$

*Remark IV.4:* For more details on the operator-theoretic approach to spectrum and to tiles, we refer to Refs. 15 and 25–27.

## V. COCYCLES IN TWO DIMENSIONS

In this section, we continue with the self-adjoint extensions of the two commuting minimal operators  $(1/i)(\partial/\partial x)$  and  $(1/i)(\partial/\partial y)$  with common dense domain  $C_c^\infty(I^2)$  in  $\mathcal{L}^2(I^2)$ .

**Theorem V.1:** *Consider two commuting unitary one-parameter groups  $U_x(s)$  and  $U_y(t)$  on  $\mathcal{L}^2(I \times I)$  with respective boundary unitaries  $U_2$  and  $V_1$ . Then:*

(i) *Either  $U_2$  is of the form  $aI_{\mathcal{L}^2(I_y)}$  for a scalar  $a$ , or else  $V_1$  commutes with periodic translation in the  $x$ -variable.*

(ii) *Either  $V_1$  is of the form  $bI_{\mathcal{L}^2(I_x)}$  for some scalar  $b$ , or else  $U_2$  commutes with periodic translation in the  $y$ -variable.*

(iii) *In case  $U_2 = e^{i2\pi\alpha} I_{\mathcal{L}^2(I_y)}$ , then*

$$U_x(s)(e_{\alpha+m} \otimes g) = e^{i2\pi(\alpha+m)s} e_{\alpha+m} \otimes g \quad (5.1)$$

for all  $m \in \mathbb{Z}$  and  $g \in \mathcal{L}^2(I_y)$ .

(iv) *In case  $V_1 = e^{i2\pi\beta} I_{\mathcal{L}^2(I_x)}$ , then*

$$U_y(t)(f \otimes e_{\beta+n}) = e^{i2\pi(\beta+n)t} f \otimes e_{\beta+n} \quad (5.2)$$

for all  $f \in \mathcal{L}^2(I_x)$  and  $n \in \mathbb{Z}$ .

*Remark V.2:* It follows that the conclusion in Theorem IV.3 is satisfied when the two one-parameter groups commute, i.e., when

$$U_x(s)U_y(t) = U_y(t)U_x(s) \quad (5.3)$$

is assumed,  $s, t \in \mathbb{R}$ . Specifically, it will then always be the case that  $U_2$  commutes with some phase-periodic translation in the  $y$ -variable, while  $V_1$  commutes with some (possibly different)

phase-periodic translation in the  $x$ -variable. [Also note that (5.3) is a reformulation of (2.3) in the case  $d=2$ . Furthermore (5.3) signifies the presence of a unitary representation of  $\mathbb{R}^2$ .]

*Proof of Theorem V.1:* When the two one-parameter groups  $U_x(s)$  and  $U_y(t)$  are written in the form (4.11) from Corollary IV.2, then the alternatives in (4.11) may be expanded as follows. Let  $\tau_s$  denote periodic translation in  $\mathcal{L}^2(\langle 0,1 \rangle)$ , and let  $P_s$  denote the projection of  $\mathcal{L}^2(\langle 0,1 \rangle)$  onto  $\mathcal{L}^2(\langle 0,s \rangle)$ , with  $P_s^\perp = I - P_s$  denoting then the projection onto the complement  $\mathcal{L}^2(\langle s,1 \rangle)$ , for  $s \in [0,1]$ . We have  $P_0=0$  and  $P_1=I_{\mathcal{L}^2(\langle 0,1 \rangle)}$ . Then from (4.11) we get

$$U_x(s) = \tau_s P_s^\perp \otimes I + \tau_s P_s \otimes U_2 \quad (5.4)$$

and

$$U_y(t) = I \otimes \tau_t P_t^\perp + V_1 \otimes \tau_t P_t. \quad (5.5)$$

The assumed commutativity (5.3) then takes the form:

$$\begin{aligned} & \tau_s P_s^\perp V_1 \otimes \tau_t P_t + \tau_s P_s \otimes U_2 \tau_t P_t^\perp + \tau_s P_s V_1 \otimes U_2 \tau_t P_t \\ &= \tau_s P_s \otimes \tau_t P_t^\perp U_2 + V_1 \tau_s P_s^\perp \otimes \tau_t P_t + V_1 \tau_s P_s \otimes \tau_t P_t U_2. \end{aligned}$$

If  $V_1$  is not a scalar times  $I_{\mathcal{L}^2(I_x)}$  then two terms on either side are independent when evaluated on  $f \otimes g$ . Hence both  $U_2 \tau_t P_t^\perp = \tau_t P_t^\perp U_2$  and  $U_2 \tau_t P_t = \tau_t P_t U_2$  hold. Addition of these two identities yields  $U_2 \tau_t = \tau_t U_2$  which is the commutativity of  $U_2$  with periodic translation.

If on the other hand  $V_1$  is a scalar, then it follows from the argument in Sec. IV that (iv) must hold.

The two possibilities for the other boundary operator  $U_2$  lead to cases (i) and (iii) by symmetry.  $\square$

*Corollary V.3:* Consider unitary one-parameter groups  $U_x(s)$  and  $U_y(t)$  as in Theorem V.1 and suppose the corresponding boundary operators  $U_2$  and  $V_1$  diagonalize as follows (identities in  $n, m \in \mathbb{Z}$ ):

$$U_2 e_{n+\beta} = e^{i2\pi\alpha_n} e_{n+\beta} \quad (5.6)$$

and

$$V_1 e_{m+\alpha} = e^{i2\pi\beta_m} e_{m+\alpha} \quad (5.7)$$

for some  $\alpha, \beta \in \mathbb{R}$ . The sequences  $\alpha_n, \beta_m$  will be chosen taking values in  $[0,1]$ . Then the commutativity (5.3) for the two groups holds if and only if the two sequences satisfy a certain cocycle property: Let  $a_n := e^{i2\pi\alpha_n}$  and  $b_m := e^{i2\pi\beta_m}$ . Then the two identities

$$(b_m - b_{m+k})(1 - a_n) = 0, \quad m, n \in \mathbb{Z}, \quad k \in \mathbb{Z} \setminus \{0\} \quad (5.8)$$

and

$$(a_n - a_{n+l})(1 - b_m) = 0, \quad m, n \in \mathbb{Z}, \quad l \in \mathbb{Z} \setminus \{0\} \quad (5.9)$$

are equivalent to the commutativity (5.3). If commutativity holds, we must have  $(1 - a_n) \cdot (1 - b_m) \equiv 0, n, m \in \mathbb{Z}$ . Hence we get a spectral pair with spectrum  $\Lambda$  having one of the two forms

$$\left\{ \begin{pmatrix} \alpha + m \\ n + \beta_m \end{pmatrix} : m, n \in \mathbb{Z} \right\} \quad \text{if } \alpha_n \equiv 0,$$

or

$$\left\{ \begin{pmatrix} m + \alpha_n \\ \beta + n \end{pmatrix} : m, n \in \mathbb{Z} \right\} \quad \text{if } \beta_m \equiv 0.$$

The derivation of the two cocycle identities (5.8) and (5.9) from commutativity (5.3) at the end of the proof is based on the following corollary of independent interest:

*Corollary V.4:* Let  $U = 1 \otimes U_2$  and  $V = V_1 \otimes I$  be the respective boundary operators of the one-parameter unitary groups  $U_x(s)$  and  $U_y(t)$  acting on  $\mathcal{L}^2(I \times I)$ . Then, if (5.6) and (5.7) hold for some  $\alpha, \beta$  and some sequences as specified, it follows that the respective one-parameter groups may be expanded in the common basis  $E(m, n) = E_{(\alpha, \beta)}(m, n) := e_{m+\alpha}^{(1)} \otimes e_{n+\beta}^{(2)}$ ,  $(m, n) \in \mathbb{Z}^2$ , as follows: There are complex sequences  $\{s_k\}_{k \in \mathbb{Z}}$  and  $\{t_l\}_{l \in \mathbb{Z}}$  so that, if we define

$$s_0^\perp := 1 - s_0, \quad t_0^\perp := 1 - t_0 \quad (5.10)$$

and

$$s_k^\perp := -s_k \quad (\text{for } k \neq 0), \quad t_l^\perp := -t_l \quad (\text{for } l \neq 0), \quad (5.11)$$

then

$$U_x(s)E(m, n) = \sum_{k \in \mathbb{Z}} e^{i2\pi(m+\alpha+k)s} (s_k^\perp + s_k a_n) E(m+k, n) \quad (5.12)$$

and

$$U_y(t)E(m, n) = \sum_{l \in \mathbb{Z}} e^{i2\pi(n+\beta+l)t} (t_l^\perp + t_l b_m) E(m, n+l). \quad (5.13)$$

The two one-parameter groups  $U_x(s)$  and  $U_y(t)$  commute if and only if the cocycle identities (5.8) and (5.9) hold.

*Proof:* Recall from (5.4) and (5.5) that the two one-parameter groups are expressed in terms of multiplication operators on  $\mathcal{L}^2(\langle 0, 1 \rangle)$  with the respective indicator functions  $\chi_{\langle 0, s \rangle}$  and  $\chi_{\langle 0, t \rangle}$ . The sequences (5.10)–(5.11) are the Fourier coefficients of these indicator functions, acting by multiplication in  $\mathcal{L}^2(I)$ , and the relations (5.10) and (5.11) simply reflect the following two obvious identities:

$$\chi_{\langle 0, s \rangle} + \chi_{[s, 1)} = 1$$

and

$$\chi_{\langle 0, t \rangle} + \chi_{[t, 1)} = 1,$$

as functions on the unit interval. When the resulting formulas (5.12) and (5.13) are substituted into

$$U_x(s)U_y(t)E(m, n) = U_y(t)U_x(s)E(m, n) \quad (5.14)$$

the equivalence to (5.8) and (5.9) results.  $\square$

## VI. QUASICRYSTALS

For the spectral pairs  $(I^d, \Lambda)$  in dimensions  $d=2, 3$ , we noted that each of the candidates for spectrum  $\Lambda$  tiles  $\mathbb{R}^d$  with  $\Lambda$ -translates of  $I^d$ . (See Theorems III.2 and IV.3.) But reviewing formulas (3.2)–(3.3) and (3.4), and (7.4) in the next section, for the possible sets  $\Lambda$  which serve as  $I^d$  spectrum, we find functions  $\alpha, \beta, \dots$  on  $\mathbb{Z}$  or  $\mathbb{Z}^k$  which describe the particular set  $\Lambda$ . Since all the candidates for  $\Lambda$  make tailings, there is a direct *geometric* interpretation for these functions; but we note in the present section that there is also a *spectral-theoretic* significance which derives from diffraction considerations of quasicrystals; see Refs. 28–30.

In this setting, diffractions show up as discrete components of the spectral distribution

$$D_{\Lambda}(x) = \sum_{\lambda \in \Lambda} e_{\lambda}(x) = \sum_{\lambda \in \Lambda} e^{i2\pi\lambda \cdot x}.$$

We say that a spectrum  $\Lambda(\subset \mathbb{R}^d)$  has a *diffraction pattern* if there is a pair  $(M, c)$  where  $M$  is a subset of  $\mathbb{R}^d$  and  $c$  is a function (measuring intensity) defined on  $M$  such that

$$D_{\Lambda}(x) = \sum_{m \in M} c(\mu) \delta(x - \mu),$$

i.e., the spectral distribution is a weighted sum of point masses, supported on some (discrete) subset  $M$  in  $\mathbb{R}^d$ . Note that the interpretation in both of the summations involving  $D_{\Lambda}(\cdot)$  is to be understood as Schwartz distributions; that is if the respective sums are evaluated on a testing function  $\varphi \in C_c^{\infty}(\mathbb{R}^d)$ , then the first sum yields  $\sum_{\lambda \in \Lambda} \tilde{\varphi}(\lambda)$  where  $\tilde{\varphi}(\lambda) = \int_{\mathbb{R}^d} e_{\lambda}(x) \varphi(x) dx$ , while the second sum is  $\sum_{\mu \in M} c(\mu) \varphi(\mu)$ . We also note that, by the Poisson summation formula, the condition is satisfied if  $\Lambda = \mathbb{Z}^d = M$ , and the density (intensity) function  $c$  is  $c \equiv 1$  on  $M$ .

We shall also need the following definition: A function  $\xi$  on  $\mathbb{R}$  is said to be *quasiperiodic* if there are positive numbers  $\omega_1, \dots, \omega_r$ , which are independent over  $\mathbb{Q}$ , and functions  $\xi_1, \dots, \xi_r$  such that  $\xi_j$  has  $\omega_j$  as period, and  $\xi = \sum_{j=1}^r \xi_j$ . The condition on  $\xi_j$  amounts to the generalized Fourier expansion

$$\xi_j(x) = \sum_{n \in \mathbb{Z}} c_j(n) \exp\left(i2\pi \frac{nx}{\omega_j}\right).$$

In the following result we show that, if the functions which define a spectrum  $\Lambda$  for some  $I^d$  are quasiperiodic, then it follows that  $\Lambda$  has a diffraction pattern. We will not state the result in the widest generality as it will be clear that the idea in the simplest case carries over to the variations in higher dimensions. Even for  $d=2$ , Theorem III.2 shows that there are two classes of  $\Lambda$  corresponding to (3.2) and (3.3), respectively. In the following we will treat only (3.2), but the result applies to (3.3) *mutatis mutandis*.

**Theorem VI.1:** *Let*

$$\Lambda = \left\{ \begin{pmatrix} m \\ \beta(m) + n \end{pmatrix} : m, n \in \mathbb{Z} \right\}$$

*for some function  $\beta: \mathbb{Z} \rightarrow \mathbb{R}$  and suppose  $\beta$  extends to a function on  $\mathbb{R}$  which is quasiperiodic with periods  $\omega_1, \dots, \omega_r$ , independent over  $\mathbb{Q}$ . Then it follows that  $(I^2, \Lambda)$  is a spectral pair with diffraction pattern, specifically, there is a density function  $c: \mathbb{Z}^r \times \mathbb{Z} \rightarrow \mathbb{C}$  such that*

$$D_{\Lambda}(x, y) = \sum_{k \in \mathbb{Z}^r} \sum_{n \in \mathbb{Z}} c(k, n) \sum_{m \in \mathbb{Z}} \delta\left(x - \sum_{i=1}^r \frac{k_i}{\omega_i} - m\right) \otimes \delta(y - n)$$

*with the density  $c(k_1, \dots, k_r, n)$  derived from the Bohr almost periodic Fourier expansion applied to  $\beta$ .*

*Proof:* Consider the formula  $D_{\Lambda}(x, y) = \sum_m \sum_n e^{i2\pi(m x + (\beta(m) + n)y)}$  and expand the inside function,  $m \mapsto e^{i2\pi\beta(m)y}$  according to the quasiperiodicity assumption on  $\beta$ : specifically,

$$\begin{aligned}
e^{i2\pi\beta(m)y} &= \prod_{j=1}^r e^{i2\pi\xi_j(m)y} \\
&= \prod_{j=1}^r \sum_{k_j \in \mathbb{Z}} c^{(j)}(k_j) \exp\left(i2\pi \frac{mk_j}{\omega_j}\right) \\
&= \sum_{k_1 \in \mathbb{Z}} \cdots \sum_{k_r \in \mathbb{Z}} c^{(1)}(k_1) \cdots c^{(r)}(k_r) \exp\left(i2\pi m \sum_{j=1}^r \frac{k_j}{\omega_j}\right).
\end{aligned}$$

Setting  $c(k) := \prod_{j=1}^r c^{(j)}(k_j)$  and using

$$\sum_{m \in \mathbb{Z}} \exp\left[i2\pi m \left(x + \sum_{j=1}^r \frac{k_j}{\omega_j}\right)\right] = \sum_{m \in \mathbb{Z}} \delta\left(x - \sum_{j=1}^r \frac{k_j}{\omega_j} - m\right)$$

together with Poisson summation (also in the second variable) we arrive at the desired formula.  $\square$

## VII. HIGHER DIMENSIONS

The following definitions help summarize the results for  $d=2$ : We say that the one-parameter unitary groups on  $\mathcal{L}^2(I \times I)$  generated by self-adjoint extensions of the respective partial derivatives  $(1/i)(\partial/\partial x)$  and  $(1/i)(\partial/\partial y)$  on  $C_c^\infty(I \times I)$  are quasicommuting if the conditions (5.6) and (5.7) hold. Recall this means that the respective boundary operators commute with some phase-periodic translation in the opposite variable. We then showed in Theorem V.1 that the commutativity property (5.3), for the unitary groups  $U_x(s)$  and  $U_y(t)$ , implies *quasicommutativity*. Finally we showed in Corollary V.3 that, among the *quasicommuting* extensions, those that in fact commute [in the sense of (5.3)] are characterized by the two cocycle identities (5.8) and (5.9).

It is clear that *quasicommutativity* can be defined analogously for  $d > 2$ . It follows from Theorem II.1 that commutativity of  $d$  self-adjoint extensions of the respective partial derivatives  $\{(1/i)(\partial/\partial x_j) : j=1, \dots, d\}$ , on  $C_c^\infty(I^d) \subset \mathcal{L}^2(I^d)$ , is equivalent to the *spectral-pair* condition for  $(I^d, \Lambda)$ . Moreover, if commuting self-adjoint extensions exist (i.e.,  $(1/i)(\partial/\partial x_j) \subset H_j$ ,  $H_j^* = H_j$ ,  $j=1, \dots, d$ ), then we may take  $\Lambda$  to be the joint spectrum of the family  $\{H_j\}_{j=1}^d$ . Conversely, commuting operators  $H_j$  may easily be associated with some spectrum  $\Lambda$  in a spectral pair  $(I^d, \Lambda)$ . Hence, for  $d=2$ , our results in Sec. V provide a complete classification of the commuting (and also the quasicommuting) self-adjoint extensions of  $\{(1/i)(\partial/\partial x_j)\}_{j=1}^d$ .

In higher dimensions, we still have boundary operators corresponding to each self-adjoint extension of the partials  $(1/i)(\partial/\partial x_j)$  (on  $C_c^\infty(I^d) \subset \mathcal{L}^2(I^d)$ ,  $j=1, \dots, d$ ), by Corollary IV.2. If for each  $j$ ,  $U_j(t)$  denotes the unitary one-parameter group on  $\mathcal{L}^2(I^d)$  generated by some self-adjoint extension  $H_j$ , then Corollary IV.2 states that  $U_j(t)$  is induced by some unitary operator  $V_j$  acting in the remaining variables  $(x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_d)$  (i.e., with omission of the variable on the  $j$ th place): specifically,  $U_j(t) = \text{ind}_{\mathbb{Z}}^{\mathbb{R}}(V_j)$  as a representation of  $(\mathbb{R}, +)$ ; or equivalently the domain of  $H_j$  is, for each  $j$ , given by the boundary condition

$$f(x_1, \dots, x_{j-1}, 1, x_{j+1}, \dots, x_d) = V_j(f(x_1, \dots, x_{j-1}, 0, x_{j+1}, \dots, x_d)).$$

(Note that the more precise interpretation of this set of boundary conditions is given in formula (4.9) of Corollary IV.2. This is the interpretation of the unitary one-parameter groups in the respective coordinate directions as *induced unitary representations* (see Refs. 31 and 32), with induction  $\mathbb{Z} \rightarrow \mathbb{R}$  for each direction.) We say that a family of self-adjoint extension operators  $H_j$ , with corresponding boundary unitaries  $V_j$ , is *quasicommuting* if there are phase angles  $\alpha_j \in [0, 1]$ ,  $j=1, \dots, d$ , such that each  $V_j$  is diagonalized by

$$e_{\alpha_1 + n_1}^{(1)} \otimes \cdots \otimes e_{\alpha_{j-1} + n_{j-1}}^{(j-1)} \otimes e_{\alpha_{j+1} + n_{j+1}}^{(j+1)} \otimes \cdots \otimes e_{\alpha_d + n_d}^{(d)} \quad (7.1)$$

as  $(n_1, \dots, n_{d-1}, n_{d+1}, \dots, n_d)$  vary over  $\mathbb{Z}^{d-1}$ , i.e., the lattice resulting from  $\mathbb{Z}^d$  with the  $j$ th coordinate place omitted. It follows that the quasicommutative case is characterized by the phase angles  $\alpha_1, \dots, \alpha_d$ , and by functions  $v_j: \mathbb{Z}^{d-1} \rightarrow \mathbb{T}$  such that, for  $n = (n_1, \dots, \hat{j}, \dots, n_d)$ ,  $v_j(n) = v_j(n_1, \dots, \hat{j}, \dots, n_d)$  is the eigenvalue of  $V_j$  corresponding to the eigenvector in (7.1). (The notation  $(n_1, \dots, \hat{j}, \dots, n_d)$  means that the  $j$ th place is omitted.)

**Theorem VII.1:** Let  $\{H_j\}_{j=1}^d$  be a family of self-adjoint extensions of the respective partials  $(1/i)(\partial/\partial x_j)$  ( $j=1, \dots, d$ , on  $C_c^\infty(I^d) \subset \mathcal{L}^2(I^d)$ ), which is assumed quasicommutative with eigenvalue functions  $v_j(n_1, \dots, \hat{j}, \dots, n_d)$  from  $\mathbb{Z}^{d-1}$  to  $\mathbb{T}$ . Then the extensions are commutative if and only if the following pair of cocycle conditions is satisfied for all  $j, k$  such that  $1 \leq j < k \leq d$ , all  $(n_1, \dots, \hat{j}, \dots, n_d)$ , and all  $l, m \in \mathbb{Z} \setminus \{0\}$ :

$$(v_j(n_1, \dots, \hat{j}, \dots, n_k + l, \dots, n_d) - v_j(n_1, \dots, \hat{j}, \dots, n_d)) \times (1 - v_k(n_1, \dots, \hat{k}, \dots, n_d)) = 0 \quad (7.2)$$

and

$$(v_k(n_1, \dots, n_j + m, \dots, \hat{k}, \dots, n_d) - v_k(n_1, \dots, \hat{k}, \dots, n_d)) \times (1 - v_j(n_1, \dots, \hat{j}, \dots, n_d)) = 0. \quad (7.3)$$

*Proof:* Since the commutativity for the one-parameter groups of unitary operators  $U_j(t_j)$  may be stated for pairs, i.e.,  $U_j(t_j)U_k(t_k) = U_k(t_k)U_j(t_j)$ ,  $j < k$ ,  $t_j \in \mathbb{R}$ ,  $t_k \in \mathbb{R}$ , the argument for the general case  $d > 2$  is the same as for  $d = 3$ . To see this, just use the formulas for the respective one-parameter groups which are analogues to (5.12) and (5.13) in the proof of Corollary V.4. For  $d = 3$ , we may introduce the leg-notation:  $v_1 \rightarrow v_{23}$ ,  $v_2 \rightarrow v_{13}$ ,  $v_3 \rightarrow v_{12}$ . When evaluated at a general point in  $\mathbb{Z}^3$  of the form  $(k, l, m)$ , the respective eigenvalues are

$$v_{23}(l, m) \quad \text{for } V_{23}, \quad (\text{i})$$

$$v_{13}(k, m) \quad \text{for } V_{13}, \quad (\text{ii})$$

$$v_{12}(k, l) \quad \text{for } V_{12}. \quad (\text{iii})$$

Specifically,

$$V_{23}e_{\beta+l}^{(2)} \otimes e_{\gamma+m}^{(3)} = v_{23}(l, m)e_{\beta+l}^{(2)} \otimes e_{\gamma+m}^{(3)}, \quad (\text{i}')$$

$$V_{13}e_{\alpha+k}^{(1)} \otimes e_{\gamma+m}^{(3)} = v_{13}(k, m)e_{\alpha+k}^{(1)} \otimes e_{\gamma+m}^{(3)}, \quad (\text{ii}')$$

$$V_{12}e_{\alpha+k}^{(1)} \otimes e_{\beta+l}^{(2)} = v_{12}(k, l)e_{\alpha+k}^{(1)} \otimes e_{\beta+l}^{(2)}, \quad (\text{iii}')$$

where  $\alpha, \beta, \gamma$  are the fixed phase angles from the quasicommutativity. Then the three pairs of cocycle identities from the theorem are as follows: (ia)–(ib), (iia)–(iib), and (iiia)–(iiib). The argument for the equivalence of commutativity and the cocycle identities is essentially the same as the one used in the proof of Corollary V.4 above. The cocycle identities for  $d = 3$  are

$$(v_{13}(k, m) - v_{13}(k + n_1, m))(1 - v_{23}(l, m)) = 0, \quad (\text{ia})$$

$$(v_{23}(l, m) - v_{23}(l + n_2, m))(1 - v_{13}(k, m)) = 0, \quad (\text{ib})$$

$$(v_{12}(k, l) - v_{12}(k + n_1, l))(1 - v_{23}(l, m)) = 0, \quad (\text{iia})$$

$$(v_{23}(l, m) - v_{23}(l, m + n_3))(1 - v_{12}(k, l)) = 0, \quad (\text{iib})$$

and

$$(v_{13}(k, m) - v_{13}(k, m + n_3))(1 - v_{12}(k, l)) = 0, \quad (\text{iiia})$$



$$(v_{12}(k, l) - v_{12}(k, l + n_2))(1 - v_{13}(k, m)) = 0. \quad (\text{iiib})$$

□

*Example VII.2:* Not all the spectral pairs in three dimensions are quasicommutative (although this is true in  $d=2$ ). Take for example the case (3.4) of Sec. III with

$$\Lambda = \left\{ \begin{pmatrix} k \\ \beta(k) + l \\ \gamma(k, l) + m \end{pmatrix} : k, l, m \in \mathbb{Z} \right\} \quad (7.4)$$

with  $\beta: \mathbb{Z} \rightarrow [0, 1)$  and  $\gamma: \mathbb{Z}^2 \rightarrow [0, 1)$  arbitrarily given functions. Then the three operators  $V_{23}$ ,  $V_{13}$ , and  $V_{12}$  are as follows:

$$V_{23} = I \text{ (the identity operator in the two marked tensor slots),} \quad (\text{i}'')$$

$$V_{13}(e_k^{(1)} \otimes e_{\gamma(k, l) + m}^{(3)}) = e^{i2\pi\beta(k)} e_k^{(1)} \otimes e_{\gamma(k, l) + m}^{(3)}, \quad (\text{ii}'')$$

and

$$V_{12}(e_k^{(1)} \otimes e_{\beta(k) + l}^{(2)}) = e^{i2\pi\gamma(k, l)} e_k^{(1)} \otimes e_{\beta(k) + l}^{(2)}. \quad (\text{iii}'')$$

It follows that the three commuting unitary one-parameter groups associated with  $\Lambda$ , via Theorem II.1, are not quasicommuting if the two functions  $\beta$  and  $\gamma$  in formula (7.4) are both nonconstant.

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